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Final Report: ONR Grant N00014-91-J-1143Unclassified: For General DistributionSteven R. White, UC Irvine
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Over the last two years, we have used several different numerical techniques to study a variety of intrinsically correlated electron systems. The three main types of numerical techniques we have used are: (1) finite-temperature quantum Monte Carlo (QMC); (2) exact diagonalization; and (3) numerical renormalization groups. We have made substantial progress both on developing and improving the numerical algorithms and in using these methods to study interesting systems. We have developed techniques for analytically continuing imaginary-time QMC data to obtain dynamical properties, and have used these techniques to study pseudogap and gap formation in the repulsive and attractive Hubbard models. We have developed a program to calculate two particle interaction vertices with full frequency and momentum dependence using QMC, and have studied possible magnetic and superconducting instabilities in the Hubbard model. We have used exact diagonalization to calculate the spectral weight function for the 4×4 Hubbard model, and to study pair-binding in small Hubbard "molecules", which may have relevance to superconductivity in fullerenes. We have developed a new momentum-space renormalization group approach, based on Wilson's numerical renormalization group for the Kondo problem, for finite Hubbard lattices. We have also discovered why previous attempts at using Wilson's approach in a real-space blocking scheme fail, and we have developed a new approach, based on density matrices, which eliminates the flaws of the old approach. When applied to Heisenberg spin chains, this approach provides results substantially better than the best available from Monte Carlo. We have used it to obtain the spatial spin density distribution of the fractional $S = 1/2$ spins at the ends of open $S = 1$ chains, as well as a variety of other properties.

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Our research over the last year has been divided roughly equally between developing and improving numerical algorithms for intrinsically correlated electron systems, and using the latest such techniques to study some of these systems. It is important for work to be done in the first area as well as the second in order for progress to continue in our understanding of these systems. While most groups use only one numerical technique, and apply it to a variety of systems, we use several completely different numerical methods. In this way we can choose the best method for each system we want to study. We have used three different numerical techniques in the last two years: (1) finite-temperature quantum Monte Carlo (QMC); (2) exact diagonalization; and (3) numerical renormalization groups. We have found that having active projects using several different methods fosters cross-pollination of ideas between the methods. For example, the new Block World-Line method currently under development by our group (described in our proposal for the next three years) combines ideas from Monte Carlo and exact diagonalization, and is related to some of the new ideas we have developed in using density matrices for numerical renormalization groups.

The quantum Monte Carlo techniques we use are excellent at computing imaginary time quantities, but it is more difficult to obtain information on dynamics. Currently the best technique to obtain dynamics from (QMC) is to use the maximum entropy method to analytically continue the QMC imaginary time data. In order to obtain high quality results, however, we found that we needed to spend some time supplementing the information contained in the QMC. (The maximum entropy method can combine a variety of sources of information in the production of an optimum fit for the spectral function). We settled on analytic moments of the spectral function as the source of additional information, and found new expressions for the first few moments for the 2D Hubbard model. We found that the information contained in the moments nicely complemented the information from QMC to produce excellent results. We have used this method to study of the single-particle spectral weight and density of states of the Hubbard model [1-4]. One of the most interesting applications to date of these techniques has been a study of the formation of gaps and pseudogaps in the spectral weight function at half-filling [2,4]. At half-filling at zero temperature, there is a well-defined antiferromagnetic gap, corresponding to long-ranged antiferromagnetic order. At high temperatures, the spin-spin correlation length is very short and this gap is not present. Schrieffer's spin bag picture for high T_c is based on a pseudogap being present when the spin-spin correlations are greater than a few lattice

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spacings. We found that a pseudogap is only present when the spin-spin correlations are comparable to the size of the lattice. At any finite temperature the correlation length is known to be finite, implying that no pseudogap is present in the infinite lattice except at $T=0$ (for moderate coupling).

We have made considerable progress in understanding exactly how to distinguish using QMC between a superconductor, an ordinary metal, and an insulator directly from the current-current correlation function for a model for which the nature of possible instabilities is unknown [5,6]. For example, ordinarily we have tested for superconductivity by looking at several pair-susceptibilities and looking for enhancement as the temperature is lowered. However, this approach has been criticized as misleading if the pair-field symmetry we choose is different from what is actually there or if the quasiparticle weight is very small. Perhaps the system would be found to have clear superconducting correlations if the physically correct pair-field operator had been guessed. By analyzing the current-current correlation function we can avoid all these possible difficulties and determine directly whether the system is superconducting (provided we can get close to the transition temperature). Using this method, we studied the positive- and negative- U Hubbard models. We found that the ground state of the half-filled positive- U Hubbard model is an insulator, the doped state is a metal (at the temperatures accessible to QMC), and the negative- U Hubbard model is a superconductor.

We have recently begun studying the two-particle scattering vertex of the Hubbard model [7,8]. This vertex is a function of three different momenta and three different frequencies, and hence has not been studied before. We have found that it is just within our current computing capabilities to calculate the vertex. The difficulty is partly because of storage requirements for such a large object and partly because the fluctuations in the two-particle vertex are larger than in simpler quantities. The vertex allows us to measure the momentum and frequency dependence of possible instabilities in both the particle-particle and particle-hole channels. By inverting the Bethe-Salpeter equation, we can study directly the irreducible vertex, and compare it with analytic approaches. If there is a superconducting instability, this approach will tell us exactly what its nature is. We have also been comparing with both the random phase approximation and third-order perturbation theory, to test approximate theories for the Hubbard model.

We have also used QMC to simulate the Holstein model [9], an electron-phonon model. This model allows us to study the competition between different types of order, such as superconductivity and charge-density-wave order. Similar types of competition occur in the high-temperature superconductors between antiferromagnetism and superconductivity.

R.N. Noack, my post-doc, came this fall with considerable expertise in the simulation of the Holstein model. We studied the effects of next-nearest neighbor hopping on the superconducting properties of the Holstein model. We found, as expected, that the superconducting transition temperature can be enhanced by the extra hopping term.

While exact diagonalization is useful only for small systems, it does not suffer from the minus sign problem. In addition, dynamical properties can be calculated exactly without use of the maximum entropy method or other analytic continuation methods. We have used this technique to calculate the spectral weight function of a 4×4 Hubbard lattice [10]. Although the computational capability has existed for several years to calculate the spectral weight for a 4×4 system, the calculation is sufficiently difficult that only very recently have there been any results reported. The results are useful for comparing both with experiments, such as angular resolved photoemission, and with QMC results using maximum entropy.

We have also used exact diagonalization to calculate pair-binding energy differences for several Hubbard systems [11]. These calculations were designed to test the ideas of Chakravarty and Kivelson on buckyball superconductivity. Chakravarty and Kivelson put forth a theory last year on superconductivity in C_{60} compounds based on a pair-binding effect on a single buckyball which they modeled with a Hubbard model. Their numerical calculations to support the theory were based on second-order perturbation theory, which left open to some question whether the effect was real. We performed exact diagonalization calculations on two small Hubbard "molecules": the 12-site truncated tetrahedron, and the 8-site cube. The truncated tetrahedron in particular has a number of similarities to the C_{60} structure. We found the pair binding effect to be present for intermediate coupling in both cases, lending support to Chakravarty and Kivelson's theory. We also found that second order perturbation theory works rather well in these systems, further supporting the theory.

The most challenging problem for QMC studies lies in finding which of many competing types of states wins out at $T=0$. This requires very low temperature studies and large lattices. Even in models with no sign problem (such as the Holstein model) getting accurate results at low enough temperatures is very challenging. For this reason we have been developing competing methods, based on Wilson's numerical renormalization group for the Kondo problem, to find ground and excited state properties of various systems. Our first attempt in this direction was based on the momentum-space representation of the Hubbard model [12]. By working in momentum space, we hoped to sidestep the well-known problems of real-space blocking approaches. We used it with fairly good results on

a 4x4 Hubbard lattice, where we could compare with exact diagonalization.

More recently we have found out how to fix the real-space blocking method so that it works for almost any lattice model [13–15]. We reformulated the old approach in terms of density matrices. We were able to show that the new approach is optimal in a certain sense, while the old approach was far from it. The approach does not require small couplings, can treat disordered systems, and of course, does not have the minus sign problem that plagues quantum Monte Carlo. This method is especially suitable for 1D problems, and we have been using it on Heisenberg spin chains, a very interesting problem for both theoretical reasons (e.g. the Haldane gap) and experimental reasons (e.g. NENP materials are modeled by these chains). The method performs *substantially* superior to any other numerical method for these chains—for example, whereas the best quantum Monte Carlo can determine the ground state energy of the infinite $S = 1$ chain to about 4 digits, this method can determine it to 9 or 10 digits. The best previous value for the Haldane gap was $\Delta = 0.41$; we have determined two more digits, $\Delta = 0.4105(1)$. We have also used it to obtain the spatial spin density distribution of the fractional $S = 1/2$ spins at the ends of open $S = 1$ chains, as well as a variety of other properties. The computational resources required for these calculations are relatively small; if extreme accuracy is not required, a modest workstation is adequate. The density matrix framework provides an important conceptual basis for all numerical RGs; for example, the zero-temperature, one-dimensional (1D), real-space algorithm we first developed could easily be generalized to finite temperature, 2D or 3D, or momentum space (although the calculations may not always be practical).

The following individuals have been supported with our ONR grant. Reinhard Noack, a former student with D. J. Scalapino at UCSB, is my postdoc. He is an expert in QMC simulations and the Holstein model, and has been involved in the renormalization group work. Guoshun Feng, a graduate student, did the exact diagonalization of a 4x4 Hubbard model, and is now working on extending the renormalization group method to the 1D Hubbard system. Marco Vekic, another graduate student, worked on the QMC simulations of the Holstein model. He is now developing a new Monte Carlo method, the block world line method mentioned above.

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